Center for Advanced Solar Photophysics
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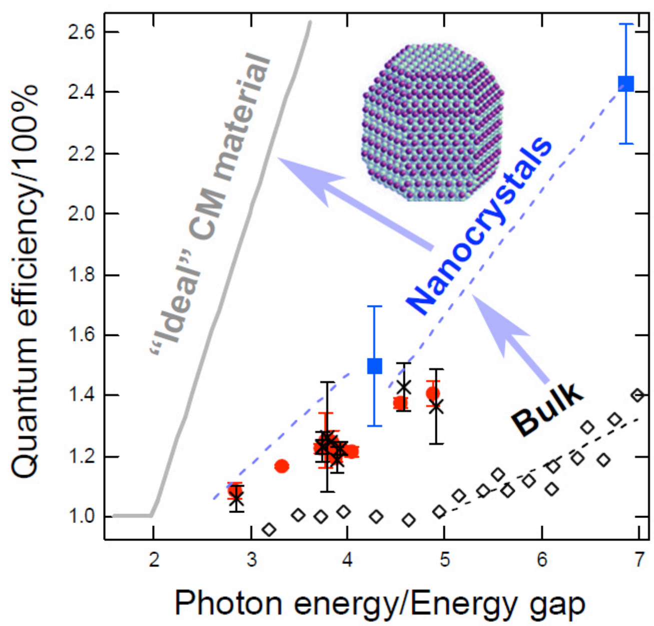
Lead Institution: Los Alamos National Laboratory

Mission Statement: The goal of this center is to explore and exploit the unique physics of nanostructured materials to boost the efficiency of solar energy conversion through novel light-matter interactions, controlled excited state dynamics, and engineered carrier-carrier coupling.

Technical Overview: Practical means to approach or *exceed* the Shockley-Queisser equilibrium thermodynamic efficiency limit require advanced mechanisms of converting photons into electrical charges. Breakthroughs in solar energy conversion are expected to come not from iterative improvements of existing technologies but instead from discoveries of new physical phenomena and/or materials with engineered functionalities. The tailorable electronic properties and unique physics of ultrasmall matter in the form of both quantum-confined semiconductors and nanostructured metals are expected to offer new processes that could yield progress toward this goal.

The research of this Center concentrates in three main Thrust areas including: 1) Novel nanoscale physical phenomena for efficient capture and conversion of light into electrical charges via quantum confinement, plasmonic and photonic effects; 2) New means for charge manipulation in nanoassemblies for rapid charge extraction and low-loss transport; 3) Proof-of-principle solar-energy conversion schemes that exploit the emergent physics of the nanoscale size regime.



Carrier multiplication in PbSe nanocrystals. Photon-to-exciton conversion efficiencies in PbSe nanocrystals compared to bulk PbS. The grey line is the "ideal" efficiency as defined by energy conservation. One goal of this center is to understand the factors that control carrier multiplication efficiency. This would allow for the development of novel nanoscale materials with performance which approaches the ideal limit.

New physical principles for light harvesting and conversion into electrical charges that will be explored in the first Thrust involve carrier multiplication (generation of multiple excitons by a single absorbed photon), engineered densities of states in plasmonic and photonic structures, band-structure engineering in nanoscale semiconductors and dynamic control of energy gap via Coulomb interactions, among others. For instance, carrier multiplication can potentially improve the power conversion efficiency of low-cost single-junction photovoltaics via production of enhanced photocurrent from blue to ultraviolet solar photons. Likewise, semiconductor-metal interactions in nanoplasmonic structures can be used to increase the absorbance of ultrathin semiconductor layers, extend the range of excitonic transfer, and tune the strength of carrier-carrier Coulomb coupling.

Effective exploitation of the unique properties of nanostructured materials in solar energy conversion, especially in utilizing multiple excitons or “hot carriers”, is contingent upon our ability to efficiently extract and transport carriers to charge collecting electrodes. The “Charge-manipulation” Thrust will explore charge separation and transport as well as energy transfer in engineered nanoassemblies. Specific previously unexplored topics will include extraction of multiple charges, exciton transport in extended gradient structures, and the effects of semiconductor-metal interaction on energy transfer.

Finally, the development of prototype Generation-III devices that demonstrate enhanced power conversion efficiency through utilization of novel nanoscale physics and architectures is a key goal of this Center. The third Thrust integrates our understanding of the unique physical principles at each step of solar energy capture and device function by developing and fabricating “exploratory” architectures. These architectures and prototype devices will be specifically designed to harness the physical principles found in both discrete and simple extended structures. Further, they will be used to elucidate key interfacial phenomena endemic to sequential increases in complexity, e.g., in progressing from a simple nanocrystal film to a multilayer device. We are focusing our studies on materials and structures amenable to scalable, low-cost fabrication and processing methodologies, such as solution-based synthesis, and on the development and refinement of compatible new techniques.

Key to each of these Thrusts is physics-driven synthesis. Promising nanoparticles and assemblies will be identified and developed based upon the most up-to-date understanding of the physics. Novel nanoparticle compositions, shapes, surface properties and hybrids will be targeted for their utility, whereas in assemblies, we will investigate novel means to functionalize and assemble materials for efficient function.

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